2008 American Control Conference
Westin Seattle Hotel, Seattle, Washington, USA
June 11-13, 2008

Reduced-Rank Unscented Kalman Filtering Using Cholesky-Based Decomposition

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I. Introduction

Data assimilation for large-scale systems has gained increasing attention due to nonlinear and computationally intensive applications such as weather forecasting [1, 2]. These problems require algorithms that are computationally tractable despite the enormous dimension of the state. Reduced-order variants of the classical Kalman filter have been developed [3, 4]. A comparison of several techniques is given in [5].

An alternative technique for reducing the computational requirements of data assimilation for high-dimensional systems is the *reduced-rank filter* [6, 7]. In this method, the error-covariance matrix is factored to obtain a square root, whose rank is then reduced through truncation. The truncated square root is then propagated by the data assimilation algorithm.

The primary technique for truncating the error-covariance matrix is the singular value decomposition (SVD), wherein the singular values are used to determine which entries of the error covariance matrix are most relevant to the accuracy of the state estimates [6, 7]. In related work [8], it is observed that the Kalman filter estimate update depends on the product C_kP_k, where C_k is the measurement map and P_k is the error covariance. In particular, it is shown in [8] that approximation of C_kP_k leads directly to truncation based on the Cholesky decomposition. Filter reduction based on the Cholesky decomposition provides state-estimation accuracy that is competitive with, and in many cases superior to, that of the SVD. An additional advantage of using the Cholesky decomposition in place of the SVD for reduced-rank filtering is the fact that the Cholesky decomposition is computationally less expensive than the SVD.

To assimilate data in nonlinear systems, particle filters are used to propagate a collection of state estimates from which statistics can be computed. These techniques include the ensemble Kalman filter (EnKF) [10, 11], which uses a stochastic construction, as well as the unscented Kalman filter (UKF) [12, 13], which deterministically constructs the collection of state estimates by perturbing the nominal state estimate. Specifically, UKF constructs the ensemble members by using the columns of the square root of the error covariance to perturb the nominal state estimate. For a model of order n, the n columns and their negatives result in $2n+1$ ensemble members and thus $2n+1$ model updates.

This research was supported by the National Science Foundation, under grants CNS-0539053 and ATM-0325332 to the University of Michigan, Ann Arbor, USA. J. Chandrasekar, I. S. Kim, and D. S. Bernstein are with The University of Michigan, Ann Arbor, MI, dsbaero@umich.edu

A straightforward approach to reducing the UKF ensemble size is to use a factorization-and-truncation method to truncate $n-q$ columns of the square root of the error covariance and construct the ensemble members using the remaining q columns. In [14], SVD-based decomposition-and-truncation is used to construct reduced-rank approximations of the square root of the error covariance, which are then used to construct the ensemble members resulting in an ensemble of size $2q+1$.

In this paper, we use the Cholesky-based decomposition technique developed in [8] to construct the reduced-ensemble members. Specifically, we use the Cholesky decomposition to obtain a square root of the error covariance and select columns of the Cholesky factor to approximate C_kP_k. The retained columns of the Cholesky factor are used to construct the ensemble members. We compare the performance of the Cholesky-decomposition-based reduced-rank UKF and the SVD-based reduced-rank UKF on a linear advection model and a nonlinear system with chaotic dynamics.

II. The Unscented Kalman Filter

We consider the discrete-time system with nonlinear dynamics

$$x_{k+1} = f(x_k, u_k, k) + w_k \tag{2.1}$$

and linearly dependent measurements

$$y_k = C_k x_k + v_k, \tag{2.2}$$

where $x_k, w_k \in \mathbb{R}^n$, $u_k \in \mathbb{R}^m$, and $y_k, v_k \in \mathbb{R}^p$. The input u_k and output y_k are assumed to be measured, and w_k and v_k are uncorrelated zero-mean white noise processes with covariances Q_k and R_k, respectively. We assume that R_k is positive definite. The objective is to obtain estimates of the state x_k using measurements y_k. When the dynamics (2.1) are linear, the Kalman filter provides estimates that minimize the mean-square-error (MSE) in the state estimates [16].

Let $x \in \mathbb{R}^n$, and let $P \in \mathbb{R}^{n\times n}$ be positive semidefinite. The unscented transformation provides $2n+1$ ensembles $X_i \in \mathbb{R}^n$ and corresponding weights $\gamma_i \in \mathbb{R}$, for $0 = 1, \ldots, 2n$, such that the weighted mean and weighted variance of the ensembles are x and P, respectively. Specifically, let $S \in \mathbb{R}^{n\times n}$ satisfy $SS^{\mathrm{T}} = P$, and, for all $i = 1, \ldots, n$, let $\mathrm{col}_i(S)$ denote the ith column of S. For $\alpha > 0$, the unscented transformation $X = \Psi(x, S, \alpha) \in \mathbb{R}^{n\times(2n+1)}$ of x with covariance $P = SS^{\mathrm{T}}$ is defined by

$$X \triangleq \left[\begin{array}{ccc} X_0 & \cdots & X_{2n} \end{array}\right], \tag{2.3}$$

where

$$X_i \triangleq \begin{cases} x, & i = 0, \\ x + \sqrt{\alpha}\mathrm{col}_i(S), & i = 1, \ldots, n, \\ x - \sqrt{\alpha}\mathrm{col}_{i-n}(S), & i = n+1, \ldots, 2n. \end{cases} \quad (2.4)$$

The parameter α determines the spread of the ensembles around x. Next, define the weights $\gamma_i \in \mathbb{R}$ by

$$\gamma_0 \triangleq \frac{\alpha - n}{\alpha}, \quad \gamma_i \triangleq \frac{1}{2\alpha}, \quad i = 1, \ldots, 2n. \quad (2.5)$$

Then,

$$\sum_{i=0}^{2n} \gamma_i X_i = x, \quad \sum_{i=0}^{2n} \gamma_i (X_i - x)(X_i - x)^{\mathrm{T}} = P. \quad (2.6)$$

UKF uses the unscented transformation to approximate the error covariance and estimate the state x_k. Letting x_0^{f} denote an initial estimate of x_0 with error covariance P_0^{f}, UKF is given by the following steps.

UKF data assimilation step:

$$x_k^{\mathrm{da}} = x_k^{\mathrm{f}} + K_k(y_k - y_k^{\mathrm{f}}), \quad (2.7)$$

$$y_k^{\mathrm{f}} = C_k x_k^{\mathrm{f}}, \quad (2.8)$$

$$X_k^{\mathrm{da}} = \Psi(x_k^{\mathrm{da}}, S_k^{\mathrm{da}}, \alpha) = \begin{bmatrix} X_{0,k}^{\mathrm{da}} & \cdots & X_{2n,k}^{\mathrm{da}} \end{bmatrix}, \quad (2.9)$$

$$S_k^{\mathrm{da}} = S_k^{\mathrm{f}} H_k^{\mathrm{f}}, \quad (2.10)$$

$$K_k = P_k^{\mathrm{f}} C_k^{\mathrm{T}} (C_k P_k^{\mathrm{f}} C_k^{\mathrm{T}} + R_k)^{-1}, \quad (2.11)$$

where $H_k^{\mathrm{f}} \in \mathbb{R}^{n \times n}$ satisfies

$$H_k^{\mathrm{f}}(H_k^{\mathrm{f}})^{\mathrm{T}} = I_n - (C_k S_k^{\mathrm{f}})^{\mathrm{T}} (C_k S_k^{\mathrm{f}} (C_k S_k^{\mathrm{f}})^{\mathrm{T}} + R_k)^{-1} C_k S_k^{\mathrm{f}} \quad (2.12)$$

and $S_k^{\mathrm{f}} \in \mathbb{R}^{n \times n}$ satisfies

$$S_k^{\mathrm{f}}(S_k^{\mathrm{f}})^{\mathrm{T}} = P_k^{\mathrm{f}}. \quad (2.13)$$

Finally, define $P_k^{\mathrm{da}} \in \mathbb{R}^{n \times n}$ by

$$P_k^{\mathrm{da}} \triangleq S_k^{\mathrm{da}} (S_k^{\mathrm{da}})^{\mathrm{T}}. \quad (2.14)$$

UKF forecast step:

$$X_{i,k+1}^{\mathrm{f}} = f(X_{i,k}^{\mathrm{da}}, u_k, k), \quad i = 0, \ldots, 2n, \quad (2.15)$$

$$x_{k+1}^{\mathrm{f}} = \sum_{i=0}^{2n} \gamma_i X_{i,k+1}^{\mathrm{f}}, \quad (2.16)$$

$$P_{k+1}^{\mathrm{f}} = \sum_{i=0}^{2n} \gamma_i \Delta X_{i,k+1}^{\mathrm{f}} (\Delta X_{i,k+1}^{\mathrm{f}})^{\mathrm{T}} + Q_k, \quad (2.17)$$

where $\Delta X_{i,k}^{\mathrm{f}} \triangleq X_{i,k}^{\mathrm{f}} - x_k^{\mathrm{f}}$. When the dynamics in (2.1) are linear, UKF is equivalent to the Kalman filter [12]. Furthermore, in the linear case, P_k^{da} and P_k^{f} are the covariances of the error $x_k - x_k^{\mathrm{da}}$ and $x_k - x_k^{\mathrm{f}}$, respectively. However, in the nonlinear case, P_k^{da} and P_k^{f} are pseudo-error covariances. The case in which the measurements depend nonlinearly on the state is discussed in [13].

Note that H_k^{f} and S_k^{f} satisfying (2.12) and (2.13) are not unique. Moreover, all square H_k^{f} and S_k^{f} satisfying (2.12) and (2.13) are related by an orthogonal transformation. Specifically, the following result is given in [18, p. 188].

Lemma 2.1: Let $S, \hat{S} \in \mathbb{R}^{n \times n}$. Then, $SS^{\mathrm{T}} = \hat{S}\hat{S}^{\mathrm{T}}$ if and only if there exists an orthogonal matrix $U \in \mathbb{R}^{n \times n}$ such that $\hat{S} = SU$.

III. SVD-Based Reduced-Rank Unscented Kalman Filter

To reduce the ensemble size, we use a reduced-rank approximation $\hat{P}_{\mathrm{s},k}^{\mathrm{f}}$ of $P_{\mathrm{s},k}^{\mathrm{f}}$. The reduced-rank approximations are chosen such that $\|\hat{P}_{\mathrm{s},k}^{\mathrm{f}} - P_{\mathrm{s},k}^{\mathrm{f}}\|_{\mathrm{F}}$ is minimized subject to $\mathrm{rank}(\hat{P}_{\mathrm{s},k}^{\mathrm{f}}) = q$, where $\|\cdot\|_{\mathrm{F}}$ denotes the Frobenius norm. Let $P \in \mathbb{R}^{n \times n}$ be positive semidefinite, let $\sigma_1 \geqslant \cdots \geqslant \sigma_n \geqslant 0$ be the singular values of P, and let $u_1, \ldots, u_n \in \mathbb{R}^n$ be the corresponding mutually orthogonal singular vectors. Next, define $U_q \in \mathbb{R}^{n \times q}$ and $\Sigma_q \in \mathbb{R}^{q \times q}$ by

$$U_q \triangleq \begin{bmatrix} u_1 & \cdots & u_q \end{bmatrix}, \quad \Sigma_q \triangleq \mathrm{diag}(\sigma_1, \ldots, \sigma_q). \quad (3.1)$$

With this notation, the singular value decomposition of P is given by $P = U_n \Sigma_n U_n^{\mathrm{T}}$, where $U_n \in \mathbb{R}^{n \times n}$ is orthogonal. For $q \leqslant n$, let $\Phi_{\mathrm{SVD}}(P, q) \in \mathbb{R}^{n \times q}$ denote the SVD-based rank-q approximation of the square root $U_n \Sigma_n^{1/2}$ of P given by $\Phi_{\mathrm{SVD}}(P, q) \triangleq U_q \Sigma_q^{1/2}$. As noted in [18], $\hat{P} = SS^{\mathrm{T}}$, where $S \triangleq \Phi_{\mathrm{SVD}}(P, q)$, is the best rank-$q$ approximation of P with respect to the Frobenius norm. The *SVD-based reduced-rank square-root unscented Kalman filter* (SVDRRUKF) is given by the following steps.

SVDRRUKF data assimilation step:

$$x_{\mathrm{s},k}^{\mathrm{da}} = x_{\mathrm{s},k}^{\mathrm{f}} + K_{\mathrm{s},k}(y_k - y_{\mathrm{s},k}^{\mathrm{f}}), \quad (3.2)$$

$$y_{\mathrm{s},k}^{\mathrm{f}} = C_k x_{\mathrm{s},k}^{\mathrm{f}}, \quad (3.3)$$

$$X_{\mathrm{s},k}^{\mathrm{da}} = \Psi_q(x_{\mathrm{s},k}^{\mathrm{da}}, S_{\mathrm{s},k}^{\mathrm{da}}, \alpha) = \begin{bmatrix} X_{\mathrm{s},0,k}^{\mathrm{da}} \cdots X_{\mathrm{s},2q,k}^{\mathrm{da}} \end{bmatrix}, \quad (3.4)$$

$$S_{\mathrm{s},k}^{\mathrm{da}} = S_{\mathrm{s},k}^{\mathrm{f}} H_{\mathrm{s},k}^{\mathrm{f}}, \quad (3.5)$$

$$K_{\mathrm{s},k} = S_{\mathrm{s},k}^{\mathrm{f}} (C_k S_{\mathrm{s},k}^{\mathrm{f}})^{\mathrm{T}} \left(C_k S_{\mathrm{s},k}^{\mathrm{f}} (C_k S_{\mathrm{s},k}^{\mathrm{f}})^{\mathrm{T}} + R_k \right)^{-1}, \quad (3.6)$$

where $H_{\mathrm{s},k}^{\mathrm{f}} \in \mathbb{R}^{q \times q}$ satisfies (2.12) with S_k^{f} replaced by $S_{\mathrm{s},k}^{\mathrm{f}}$.

SVDRRUKF forecast step:

$$X_{\mathrm{s},i,k+1}^{\mathrm{f}} = f(X_{\mathrm{s},i,k}^{\mathrm{da}}, u_k, k), \quad i = 0, \ldots, 2q, \quad (3.7)$$

$$x_{\mathrm{s},k+1}^{\mathrm{f}} = \sum_{i=0}^{2q} \gamma_{q,i} X_{\mathrm{s},i,k+1}^{\mathrm{f}}, \quad (3.8)$$

$$P_{\mathrm{s},k+1}^{\mathrm{f}} = \sum_{i=0}^{2q} \gamma_{q,i} \Delta X_{\mathrm{s},i,k+1}^{\mathrm{f}} (\Delta X_{\mathrm{s},i,k+1}^{\mathrm{f}})^{\mathrm{T}} + Q_k, \quad (3.9)$$

$$S_{\mathrm{s},k+1}^{\mathrm{f}} = \Phi_{\mathrm{SVD}}(P_{\mathrm{s},k+1}^{\mathrm{f}}, q). \quad (3.10)$$

where $\Delta X_{\mathrm{s},i,k}^{\mathrm{f}} \triangleq X_{\mathrm{s},i,k}^{\mathrm{f}} - x_{\mathrm{s},k}^{\mathrm{f}}$.

Next, define $\hat{P}_{\mathrm{s},k}^{\mathrm{f}}, \hat{P}_{\mathrm{s},k}^{\mathrm{da}} \in \mathbb{R}^{n \times n}$ by

$$\hat{P}_{\mathrm{s},k}^{\mathrm{f}} \triangleq S_{\mathrm{s},k}^{\mathrm{f}} (S_{\mathrm{s},k}^{\mathrm{f}})^{\mathrm{T}}, \quad \hat{P}_{\mathrm{s},k}^{\mathrm{da}} \triangleq S_{\mathrm{s},k}^{\mathrm{da}} (S_{\mathrm{s},k}^{\mathrm{da}})^{\mathrm{T}}. \quad (3.11)$$

It then follows from (3.5) that

$$\hat{P}_{\mathrm{s},k}^{\mathrm{da}} = \hat{P}_{\mathrm{s},k}^{\mathrm{f}} - \hat{P}_{\mathrm{s},k}^{\mathrm{f}} C_k^{\mathrm{T}} (C_k \hat{P}_{\mathrm{s},k}^{\mathrm{f}} C_k^{\mathrm{T}} + R_k)^{-1} C_k \hat{P}_{\mathrm{s},k}^{\mathrm{f}}. \quad (3.12)$$

Furthermore, (3.6) and (3.12) imply that

$$K_{\mathrm{s},k} = \hat{P}_{\mathrm{s},k}^{\mathrm{f}} C_k^{\mathrm{T}} (C_k \hat{P}_{\mathrm{s},k}^{\mathrm{f}} C_k^{\mathrm{T}} + R_k)^{-1}. \quad (3.13)$$

Since the SVD in (3.10) is computationally intensive [9], we introduce an alternative method to obtain a reduced-rank approximation of a square root of the pseudo-error covariance.

IV. Cholesky-Decomposition-Based Reduced-Rank Unscented Kalman Filter

The filter gain K_k of UKF depends on a particular subspace of the forecast error covariance P_k^{f}. Specifically, K_k depends only on the correlation $C_kP_k^{\mathrm{f}}$ between the error in the measured states and unmeasured states. Since $\mathrm{rank}(C_k) = p$, there exists a state space basis with respect to which C_k has the form

$$C_k = \left[\begin{array}{cc} I_p & 0 \end{array}\right]. \tag{4.1}$$

The following result is given in [8].

Lemma 4.1: Partition P_k^{f} as

$$P_k^{\mathrm{f}} = \left[\begin{array}{cc} P_{p,k}^{\mathrm{f}} & (P_{\overline{p}p,k}^{\mathrm{f}})^{\mathrm{T}} \\ P_{\overline{p}p,k}^{\mathrm{f}} & P_{\overline{p},k}^{\mathrm{f}} \end{array}\right], \tag{4.2}$$

where $P_{p,k}^{\mathrm{f}} \in \mathbb{R}^{p\times p}$ and $P_{\overline{p},k}^{\mathrm{f}} \in \mathbb{R}^{\overline{p}\times\overline{p}}$, and assume that C_k has the form (4.1). Then,

$$K_k = \left[\begin{array}{c} P_{p,k}^{\mathrm{f}} \\ P_{\overline{p}p,k}^{\mathrm{f}} \end{array}\right](P_{p,k}^{\mathrm{f}} + R_k)^{-1}. \tag{4.3}$$

To reduce the ensemble size, we construct a filter that uses a reduced-rank approximation $\hat{P}_{\mathrm{c},k}^{\mathrm{f}}$ of $P_{\mathrm{c},k}^{\mathrm{f}}$ such that $\mathrm{rank}(\hat{P}_{\mathrm{c},k}^{\mathrm{f}}) < n$ and $\|C_k(\hat{P}_{\mathrm{c},k}^{\mathrm{f}} - P_{\mathrm{c},k}^{\mathrm{f}})\|_{\mathrm{F}}$ is minimized. To obtain $\hat{P}_{\mathrm{c},k}^{\mathrm{f}}$, we perform a Cholesky decomposition of the pseudo-error covariance $P_{\mathrm{c},k}^{\mathrm{f}}$ at each time step. Assuming that $P \in \mathbb{R}^{n\times n}$ is positive definite, the Cholesky decomposition of P yields a unique lower triangular Cholesky factor $L \in \mathbb{R}^{n\times n}$ satisfying

$$LL^{\mathrm{T}} = P. \tag{4.4}$$

Truncating the last $n-q$ columns of $L = \left[\begin{array}{ccc} L_1 & \cdots & L_n \end{array}\right]$ yields the rank-q Cholesky factor

$$\Phi_{\mathrm{CHOL}}(P,q) \triangleq \left[\begin{array}{ccc} L_1 & \cdots & L_q \end{array}\right] \in \mathbb{R}^{n\times q}. \tag{4.5}$$

The following result is given in [8].

Lemma 4.2: Let $P \in \mathbb{R}^{n\times n}$ be positive definite, define $S \triangleq \Phi_{\mathrm{CHOL}}(P,q)$, where $0 < q \leqslant n$, and partition P and $\hat{P} \triangleq SS^{\mathrm{T}}$ as

$$P = \left[\begin{array}{cc} P_q & P_{q\overline{q}} \\ (P_{q\overline{q}})^{\mathrm{T}} & P_{\overline{q}} \end{array}\right], \quad \hat{P} = \left[\begin{array}{cc} \hat{P}_q & \hat{P}_{q\overline{q}} \\ (\hat{P}_{q\overline{q}})^{\mathrm{T}} & \hat{P}_{\overline{q}} \end{array}\right], \tag{4.6}$$

where $P_q, \hat{P}_q \in \mathbb{R}^{q\times q}$ and $P_{\overline{q}}, \hat{P}_{\overline{q}} \in \mathbb{R}^{\overline{q}\times\overline{q}}$. Then,

$$\left[\begin{array}{cc} \hat{P}_q & \hat{P}_{q\overline{q}} \end{array}\right] = \left[\begin{array}{cc} P_q & P_{q\overline{q}} \end{array}\right]. \tag{4.7}$$

Lemma 4.2 implies that, if $S = \Phi_{\mathrm{CHOL}}(P,q)$, then the first q columns and rows of SS^{T} and P are equal. The *Cholesky-decomposition-based reduced-rank unscented Kalman filter* (CDRRUKF) is summarized as follows.

CDRRUKF data assimilation step:

$$x_{\mathrm{c},k}^{\mathrm{da}} = x_{\mathrm{c},k}^{\mathrm{f}} + K_{\mathrm{c},k}(y_k - y_{\mathrm{c},k}^{\mathrm{f}}), \tag{4.8}$$

$$y_{\mathrm{c},k}^{\mathrm{f}} = C_k x_{\mathrm{c},k}^{\mathrm{f}}, \tag{4.9}$$

$$X_{\mathrm{c},k}^{\mathrm{da}} = \Psi_q(x_{\mathrm{c},k}^{\mathrm{da}}, S_{\mathrm{c},k}^{\mathrm{da}}, \alpha), \tag{4.10}$$

$$S_{\mathrm{c},k}^{\mathrm{da}} = S_{\mathrm{c},k}^{\mathrm{f}} H_{\mathrm{c},k}^{\mathrm{f}}, \tag{4.11}$$

$$K_{\mathrm{c},k} = S_{\mathrm{c},k}^{\mathrm{f}}(C_kS_{\mathrm{c},k}^{\mathrm{f}})^{\mathrm{T}}\left(C_kS_{\mathrm{c},k}^{\mathrm{f}}(C_kS_{\mathrm{c},k}^{\mathrm{f}})^{\mathrm{T}} + R_k\right)^{-1}, \tag{4.12}$$

where $H_{\mathrm{c},k}^{\mathrm{f}} \in \mathbb{R}^{q\times q}$ satisfies (2.12) with S_k^{f} replaced by $S_{\mathrm{c},k}^{\mathrm{f}}$.

CDRRUKF forecast step:

$$X_{\mathrm{c},i,k+1}^{\mathrm{f}} = f(X_{\mathrm{c},i,k}^{\mathrm{da}}, u_k, k), \quad i = 0, \ldots, 2q \tag{4.13}$$

$$x_{k+1}^{\mathrm{f}} = \sum_{i=0}^{2q} \gamma_{q,i} X_{\mathrm{c},i,k+1}^{\mathrm{f}}, \tag{4.14}$$

$$P_{\mathrm{c},k+1}^{\mathrm{f}} = \sum_{i=0}^{2q} \gamma_{q,i} \Delta X_{\mathrm{c},i,k+1}^{\mathrm{f}} (\Delta X_{\mathrm{c},i,k+1}^{\mathrm{f}})^{\mathrm{T}} + Q_k, \tag{4.15}$$

$$S_{\mathrm{c},k+1}^{\mathrm{f}} = \Phi_{\mathrm{CHOL}}(P_{\mathrm{c},k+1}^{\mathrm{f}}, q), \tag{4.16}$$

where $\Delta X_{\mathrm{c},i,k}^{\mathrm{f}} = X_{\mathrm{c},i,k}^{\mathrm{f}} - x_{\mathrm{c},k}^{\mathrm{f}}$.

Next, define $\hat{P}_{\mathrm{c},k}^{\mathrm{da}}, \hat{P}_{\mathrm{c},k}^{\mathrm{f}} \in \mathbb{R}^{n\times n}$ by $\hat{P}_{\mathrm{c},k}^{\mathrm{f}} \triangleq S_{\mathrm{c},k}^{\mathrm{f}}(S_{\mathrm{c},k}^{\mathrm{f}})^{\mathrm{T}}$ and

$$\hat{P}_{\mathrm{c},k}^{\mathrm{da}} \triangleq \hat{P}_{\mathrm{c},k}^{\mathrm{f}} - \hat{P}_{\mathrm{c},k}^{\mathrm{f}} C_k^{\mathrm{T}}(C_k\hat{P}_{\mathrm{c},k}^{\mathrm{f}}C_k^{\mathrm{T}} + R_k)^{-1} C_k \hat{P}_{\mathrm{c},k}^{\mathrm{f}}. \tag{4.17}$$

It then follows from (4.11) that $S_{\mathrm{c},k}^{\mathrm{da}}(S_{\mathrm{c},k}^{\mathrm{da}})^{\mathrm{T}} = \hat{P}_{\mathrm{c},k}^{\mathrm{da}}$. Furthermore, (4.12) and (4.17) imply that

$$K_{\mathrm{c},k} = \hat{P}_{\mathrm{c},k}^{\mathrm{f}} C_k^{\mathrm{T}}(C_k\hat{P}_{\mathrm{c},k}^{\mathrm{f}}C_k^{\mathrm{T}} + R_k)^{-1}. \tag{4.18}$$

Hence, like the estimator gain $K_{\mathrm{s},k}$ of SVDRRUKF, the estimator gain $K_{\mathrm{c},k}$ of CDRRUKF depends on a reduced-rank approximation $\hat{P}_{\mathrm{c},k}^{\mathrm{f}}$ of the pseudo-error covariance $P_{\mathrm{c},k}^{\mathrm{f}}$. Due to the rank-reduction step (4.16), CDRRUKF is generally not equivalent to UKF. However, we now discuss cases in which the performance of CDRRUKF is close to that of UKF.

A. Basis Selection for CDRRUKF

The following result given in [8] shows that CDRRUKF is equivalent to UKF for a single time step when C_k has the form (4.1).

Proposition 4.1: Assume that $p \leqslant n$, $q = p$, and C_k has the structure in (4.1). Let $P_k^{\mathrm{f}} \in \mathbb{R}^{n\times n}$ be positive semidefinite and K_k be given by (2.11). Furthermore, define $S_{\mathrm{c},k}^{\mathrm{f}} \triangleq \Phi_{\mathrm{CHOL}}(P_k^{\mathrm{f}}, q)$ and let $\hat{P}_{\mathrm{c},k}^{\mathrm{f}}$ be given by (4.17). Then, $C_k\hat{P}_{\mathrm{c},k}^{\mathrm{f}} = C_kP_k^{\mathrm{f}}$ and hence, $K_{\mathrm{c},k} = K_k$.

If the dynamics (2.1) are linear and time-invariant, that is, for all $k \geqslant 0$,

$$x_{k+1} = Ax_k + Bu_k + w_k, \tag{4.19}$$

$$y_k = Cx_k + v_k, \tag{4.20}$$

then a basis for the state x can be chosen so that CDRRUKF is equivalent to UKF for $r > 0$ time steps. To construct such a basis, we define the observability matrix $\mathcal{O}(A,C) \in \mathbb{R}^{pn\times n}$ by

$$\mathcal{O}(A,C) \triangleq \left[\begin{array}{cccc} C^{\mathrm{T}} & (CA)^{\mathrm{T}} & \cdots & (CA^{n-1})^{\mathrm{T}} \end{array}\right]^{\mathrm{T}}. \tag{4.21}$$

The following result is given in [8].

Proposition 4.2: Assume that $\mathcal{O}(A,C)$ has the form

$$\mathcal{O}(A,C) = \left[\begin{array}{c} I_n \\ 0_{(p-1)n\times n} \end{array}\right]. \tag{4.22}$$

Let $r > 0$ be an integer such that $pr < n$, and let $q = pr$. Furthermore, assume that $P_{\mathrm{c},0}^{\mathrm{f}} = P_0^{\mathrm{f}}$. Then, for all $k = 0, \ldots, r$, $K_{\mathrm{c},k} = K_k$. If, in addition, $x_{\mathrm{c},0}^{\mathrm{f}} = x_0^{\mathrm{f}}$, then for all $k = 0, \ldots, r$, $x_{\mathrm{c},k}^{\mathrm{f}} = x_k^{\mathrm{f}}$.

Let x_k have entries $x_k = \left[\begin{array}{ccc} x_{1,k} & \cdots & x_{n,k} \end{array}\right]^{\mathrm{T}}$. If $\mathcal{O}(A,C)$ has the form (4.22), and $u_k = w_k = v_k = 0$,

for all $k \geqslant 0$, then for all $k \geqslant 0$, and for every integer $r > 0$ such that $pr \leqslant n$,

$$\begin{bmatrix} y_k^{\mathrm{T}} & \cdots & y_{k+r-1}^{\mathrm{T}} \end{bmatrix}^{\mathrm{T}} = \begin{bmatrix} x_{1,k}^{\mathrm{T}} & \cdots & x_{pr,k}^{\mathrm{T}} \end{bmatrix}^{\mathrm{T}}. \tag{4.23}$$

Next, we consider the nonlinear system (2.1) and assume that the dynamics in (2.1) can be expressed as

$$x_{i,k+1} = f_i(x_{\phi_{\mathrm{L}}(i,b)}, \ldots, x_{\phi_{\mathrm{R}}(i,b)}, u_k, k) + w_{i,k}, \tag{4.24}$$

where $i = 1, \ldots, n$, $b > 0$ and

$$\phi_{\mathrm{L}}(i,b) \triangleq \max(1, i-b), \quad \phi_{\mathrm{R}}(i,b) \triangleq \min(n, i+b). \tag{4.25}$$

For example, in systems modeled by finite volume schemes, the next value of a physical variable in a given cell depends only on the present values of the physical variables in its neighboring cells.

Next, let y_k denote a measurement of a specific component of the state, so that $y_k = x_{j,k} + v_k$, where $j \in \{1, \ldots, n\}$, $j - rb \geqslant 1$, and $j + rb \leqslant n$. It follows from (4.24) that, if $w_k = v_k = 0$, for all $k \geqslant 0$, then $y_k, \ldots, y_{k+r-1}$ depends on only first $2rb$ components of the state vector $\tilde{x}_k$ at time step k. Hence, a state space basis can be chosen such that the outputs $y_k, \ldots, y_{k+r-1}$ depend on only the first few components of the state vector.

V. Linear Advection Model

Consider a linear advection model [2] with n cells, and let $x_{i,k}$ be the energy in the ith cell at time k. The energy flow satisfies

$$x_{i,k+1} = \begin{cases} x_{i-1,k}, & \text{if } i = 2, \ldots, n, \\ x_{n,k}, & \text{if } i = 1. \end{cases} \tag{5.1}$$

Hence, energy in the ith cell flows to the $(i+1)$th cell, while the periodic boundary condition ensures that the energy circulates continually. We choose $n = 100$ and assume that the disturbance w_k enters selected cells, where $w_k \in \mathbb{R}^n$ is a white noise process with covariance $Q_k = Q$ for all $k \geqslant 0$, and $Q \in \mathbb{R}^{n \times n}$ is diagonal with nonzero entries $Q_i = 1$ only for $i \in \{10, 20, \ldots, 100\}$. Next, we assume that measurements of the energy in cells 50 and 51 are available so that $y_k = [x_{50,k} \;\; x_{51,k}]^{\mathrm{T}} + v_k$, where v_k is white noise process with covariance $R_k = 0.1 I_2$.

First, we use the measurements y_k to estimate the energy in the remaining cells using UKF. In all three cases, the initial estimates x_0^{f}, $x_{\mathrm{s},0}^{\mathrm{f}}$, and $x_{\mathrm{c},0}^{\mathrm{f}}$ are not equal to the initial state x_0. Moreover, we choose $P_0^{\mathrm{f}} = P_{\mathrm{s},0}^{\mathrm{f}} = P_{\mathrm{c},0}^{\mathrm{f}} = 0.1 I_n$. Finally, we choose $\alpha = 0.6$ for all three filters.

As shown in Figure 1 and Figure 2, data assimilation is performed using SVDRRUKF and CDRRUKF for several values of q between 5 and 100. It can be seen that the performance of SVDRRUKF with 111 ensemble members ($q = 55$) is close to optimal, whereas the performance of CDRRUKF is close to optimal with 11 ensemble members ($q = 5$). The steady-state MSE of state estimates for various values of q is plotted in Figure 3 and Figure 4. The performance of SVDRRUKF is poor when $q < 55$, and close to optimal when $q \geqslant 55$. Thus the ensemble size can be reduced from 201 to 111 with negligible change in the performance. However, the ensemble size can be reduced from 211 to 11 with negligible performance deterioration.

Next, we repeat the same procedure except with a poor estimate of the process noise covariance for data assimilation. Specifically, we replace Q_k in (3.9) and (4.15) by $\hat{Q}_k$, where $\hat{Q}_k = I$ for all $k \geqslant 0$. The steady-state MSE of state estimates for different choices of q is plotted in Figure 3 and Figure 4. SVDRRUKF with a poor estimate of the error covariance is unstable for all $q \leqslant 95$ (indicated by the X's). However, Figure 4 shows that even with $q = 5$ and a poor estimate of the process noise covariance, the performance of CDRRUKF is close to optimal.

Finally, we replace Q_k in (4.16) with $\hat{Q}_k$, where $\hat{Q}_k = \alpha I$ for all $k \geqslant 0$, and perform state estimation using CDRRUKF. The steady-state MSE of the state estimates is shown in Figure 5 for several values of α. For all the cases, the performance of CDRRUKF is close to optimal when $\alpha \geqslant 1$. This suggests that it is advantageous to overestimate the process noise covariance. SVDRRUKF is unstable for all choices of $\alpha = 0.005, \ldots, 50$. Hence, these simulations suggest that CDRRUKF is more robust than SVDRRUKF with respect to uncertainties in the process noise covariance. All of the results for CDRRUKF in figures 1-6 are obtained using a state space basis with respect to which the observability matrix has the form (4.22).

VI. L96 Model

The L96 model mimics the propagation of an unspecified meteorological quantity along a latitude circle [17]. The dynamics are governed by

$$\frac{d}{dt} x_i(t) = (x_{i+1}(t) - x_{i-2}(t)) x_{i-1}(t) - x_i(t) + u_i(t), \tag{6.1}$$

where $x_i(t) \in \mathbb{R}$ denotes the meteorological quantity at the ith grid point at time t, $u_i \in \mathbb{R}$ denotes an external forcing term, and w_i denotes unknown disturbances affecting the ith grid point. For all $t \geqslant 0$, the boundary conditions are defined by $x_0(t) = x_n(t)$, $x_{-1}(t) = x_{n-1}(t)$, $x_{n+1}(t) = x_1(t)$. We choose $u_i(t) = 8$ for all $i = 1, \ldots, n$ and all $t \geqslant 0$. Using fourth-order Runge-Kutta discretization with a sampling time of 0.05 s, we obtain a discrete-time model of (6.1) that can be expressed as (2.1). Furthermore, we assume that the discretized model is corrupted by an unknown external disturbance that affects specified cells. We choose $n = 40$, and assume that w_k is white noise process with covariance $Q_k = Q$ for all $k \geqslant 0$, where $Q \in \mathbb{R}^{n \times n}$ is diagonal with nonzero entries $Q_{i,i} = 0.1$ only for $i \in \{5, 15, 25, 35\}$. Next, we assume that measurements from cells with 20 and 21 are available so that $y_k = [x_{20,k} \; x_{21,k}]^{\mathrm{T}} + v_k$, where v_k is white noise process with covariance $R_k = 0.01 I_2$.

We use the measurements y_k to estimate the state in the cells where measurements are not available. Next, as shown in Figure 6 and Figure 7, we reduce the ensemble size and use SVDRRUKF and CDRRUKF with $q = 10, 20, 30$. It can be seen that the performance of SVDRRUKF is poor compared to the performance of CDRRUKF for both $q = 20$ and $q = 30$. Moreover, the performance of CDRRUKF with

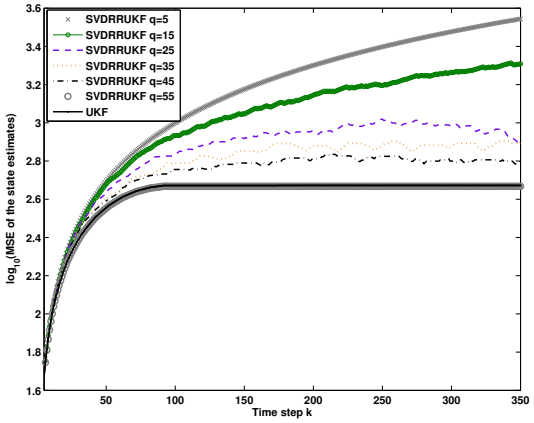

Fig. 1. MSE of the state estimates obtained from SVDRRUKF for several values of q. SVDRRUKF with $q = 5$ is unstable, while the performance of SVDRRUKF with $q = 55$ is close to the performance of full-order UKF.

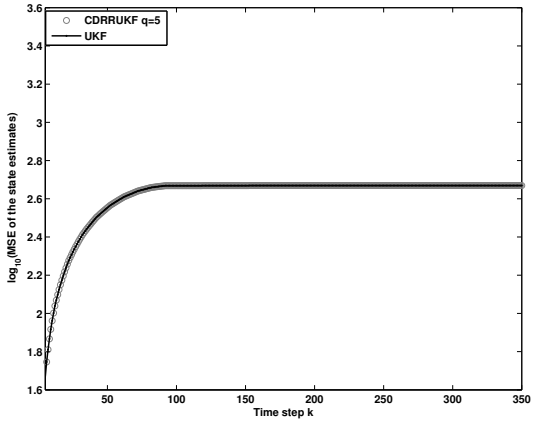

Fig. 2. MSE of the state estimates obtained from CDRRUKF with $q = 5$. The performance of CDRRUKF with $q = 5$ is close to the full-order UKF performance.

61 ($q = 30$) ensemble members is close to the performance of UKF with 81 ensemble members.

Next, we replace Q_k in (3.9) and (4.15) by $\hat{Q}_k$, where $\hat{Q}_k = \alpha I$ for all $k \geqslant 0$. Figure 8 shows the time-averaged MSE of state estimates obtained using SVDRRUKF and CDRRUKF with $q = 10$ and $q = 20$ for several values of α between 0.001 and 100. It can be seen that, for all values of α, the performance of CDRRUKF is superior to the performance of SVDRRUKF. In fact, CDRRUKF with 21 ensemble members ($q = 10$) consistently outperforms SVDRRUKF with 41 ensemble members ($q = 20$). Finally, note that (6.1) can be expressed as (4.24) with $b = 1$. All of the results for CDRRUKF in figures 8-12 are obtained using the state space basis discussed in Section IV-A.

VII. Conclusions

We developed a reduced-rank square-root unscented Kalman filter based on the Cholesky decomposition of the pseudo-error covariance. We compare the performance of the Cholesky-based filter with an analogous filter that uses the singular value decomposition for a linear advection model and a nonlinear system that exhibits chaotic behavior. Although the computational requirement of the Cholesky-based reduced-rank filter is less than that of the SVD-based reduced-rank filter, the results presented here suggest that the estimation accuracy of the Cholesky-based reduced-rank filter is significantly better than that of SVD-based reduced-rank filter. Moreover, simulation results suggest that the Cholesky-based reduced-rank filter is more robust to uncertainties in the process noise covariance than the SVD-based reduced-rank filter.

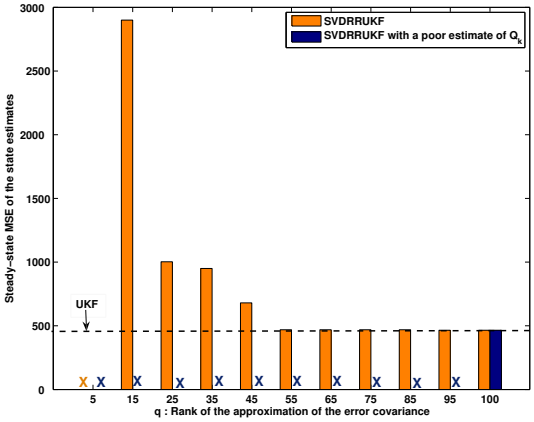

Fig. 3. Steady-state performance of SVDRRUKF. For each value of q, we perform data assimilation with the true value of the process noise covariance and with a poor estimate of the process noise covariance. The X's indicate cases in which the filter is unstable.

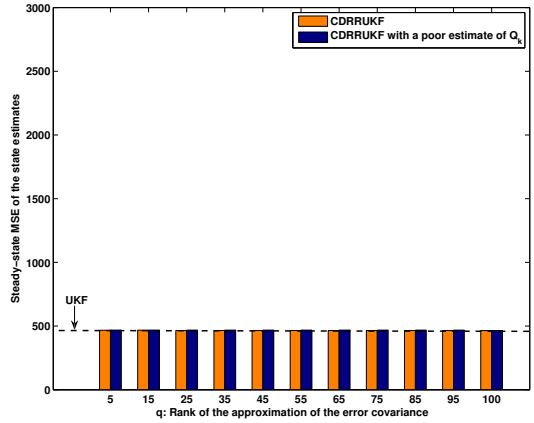

Fig. 4. Steady-state performance of CDRRUKF for values of q between 5 and 100. Note that for $q = 5$, the performance of CDRRUKF is close to optimal, irrespective of the value of the process noise covariance used for data assimilation.

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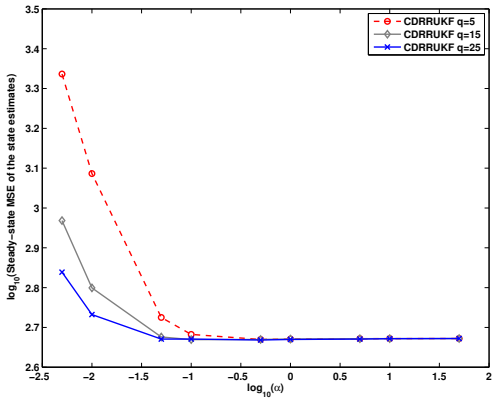

Fig. 5. Steady-state performance of CDRRUKF with $q = 5, 15, 25$. In all three cases, we use a poor estimate of the process noise covariance for data assimilation. For a fixed level of uncertainty in the process noise covariance, the performance of CDRRUKF improves when the ensemble size increases. The performance of SVDRRUKF is not shown since SVDRRUKF is unstable for all values of α and $q = 5, 15, 25$.

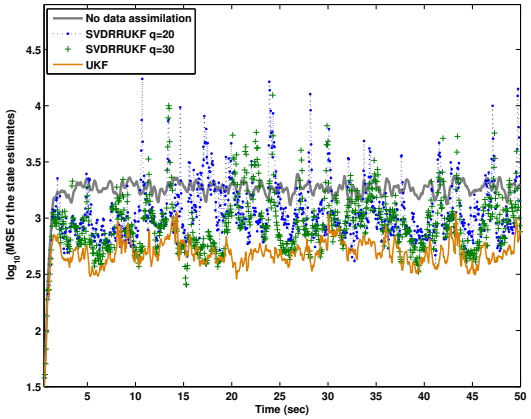

Fig. 6. MSE of the state estimates obtained using SVDRRUKF with $q = 20, 30$. The error in state estimates based on UKF and data-free simulation is shown for comparison. SVDRRUKF with $q = 20$ and $q = 30$ sometimes yields estimates that are worse than estimates based on data-free simulation.

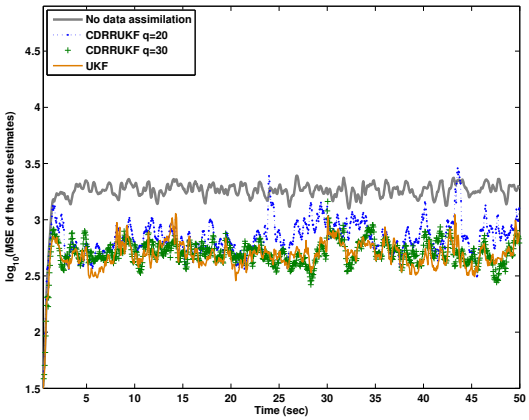

Fig. 7. Performance of CDRRUKF with $n = 40$ and $q = 20, 30$. Note that the performance of CDRRUKF with $q = 20$ is better than the performance of SVDRRUKF with $q = 30$.

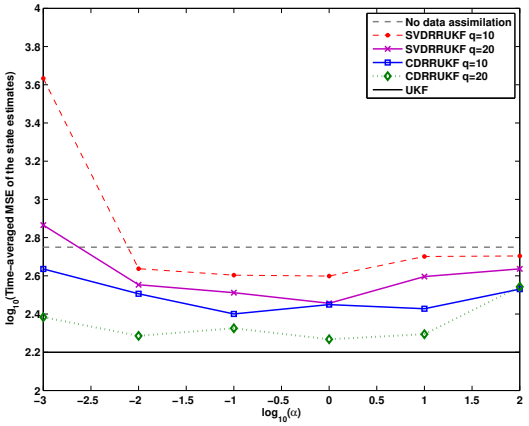

Fig. 8. Time-averaged MSE of state estimates between 35 sec and 50 sec. The state estimates are obtained using SVDRRUKF and CDRRUKF with $q = 10$ and $q = 20$, and a poor estimate of the process noise covariance. For all values of α, the performance of CDRRUKF is better than the performance of SVDRRUKF.

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